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A novel multiphase DNS method for the resolution of Brownian motion in a weakly rarefied gas using a continuum framework

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Abstract

In this paper, we formulate an Immersed boundary based direct numerical simulation (DNS) technique for resolving the particle-fluid coupling between a nano-particle and a (weakly) rarefied gas. Such a method resolves the mobility of these solid particles by incorporating the hydrodynamics of the fluid more rigorously within the conventional Langevin description of the system. We analyse the consequences of resolving the subsequent Brownian motion of spherical soot-like hydrocarbon (HC) nano-particles in an unbounded domain using such a framework. The proposed method is able to capture the transition from a particle-inertia dominated (highly correlated) ballistic regime (t^2) to a non-correlated diffusive one ($2Dt$ as given by the Stokes-Einstein relation) and further accurately estimate the resulting diffusivity of the nano-particle. This method can be used within any multiphase DNS framework to reproduce the meandering motion of soot-like Brownian particles under similar conditions.

Introduction

The physical laws governing transport of nano-particles in a gas (aerosols) may differ from their macroscopic counterpart in that non-continuum effects become more pronounced, i.e. the particles no longer experience the carrier phase as a continuum but would rather collide with its constitutive molecules or atoms. This results in two primary effects, firstly there is a reduced momentum transfer between the particle and fluid (sometimes described as the occurrence of a slip velocity at the particle surface), and secondly the existence of a meandering particle trajectory (commonly referred to as Brownian motion) due to the incessant regular molecular collisions. A comprehensive resolution of the non-equilibrium rarefied dynamics can be achieved by directly solving the kinetic equations that govern such a system, however these are extremely time and memory consuming at the limit of weakly rarefied flows. Further, other coarse-grained (such as dissipative particle dynamics) and hybrid methods are still not realizable at larger system scales particularly due to the complexities involved in the gas-solid coupling. There is thus a noticeable need for a numerical method that can handle practical gas-solid rarefied flows at reasonable computational loads.

Hence in this paper, we present a simulation tool that extends the applicability of a fully resolved continuum description (DNS) of a weakly rarefied gas to describe the dispersion of soot-like spherical nano-particles in an unbounded domain.

Numerical method: IB-FSI framework

The fundamental idea behind this framework is to couple the extended stochastic Langevin description (1) with an Immersed boundary (IB) method (Mark, Rundqvist & Edelvik 2011). This framework employs the empirical Cunningham correction (C_c) to account for the drag reduction due to rarefaction (non-continuum behaviour).

$$m_p \frac{du}{dt} = \frac{F_{Hydrodynamic}}{C_c} + F_{Brownian} \tag{1}$$

In our framework, the resolved hydrodynamic forces ($F_{Hydrodynamic}$) are used instead of the traditionally employed Stokes-based quasi-steady models (Ounis & Ahmadi 1990). The IB solver used in this work (IPS IBOFlow®) solves the governing equations on an octree grid, that is dynamically refined around the moving body to resolve the local stresses. To get the total hydrodynamic force, the fluid stresses are integrated over the surface. Further, the Brownian perturbations ($F_{Brownian}$) , which are imposed on the particle surface, are modelled as a Gaussian white noise process (Chandrasekhar 1943). The resulting rigid body motion is solved by a finite element based solver (Simo & Wong 1991). For a more detailed description of the framework and some conclusive validations, see (Mark, Rundqvist & Edelvik 2011).

Results and Discussion

The Ounis and Ahmadi model (Eq.1), including the fully resolved hydrodynamic coupling (from the IB method), is used to study the diffusion of a single spherical HC nano-particle (of diameter *dp* 400 nm) in air within an unbounded domain. A minimum spatial resolution of 24 cells/diameter and a temporal resolution much lesser than the particle response time ($\tau_p/200$) is maintained in the numerical setup in order to ensure convergence. Further, the Brownian fluctuations are enforced every $\tau_p/10$ timesteps to allow for a better resolution of the stochastic coupling. A single long realization of the stochastic process (100 particle response times) is used to estimate the relevant statistics. The Figs. 1a and b show the general schematic of the simulation domain including the spatial resolution around the particle. A general Brownian trajectory of a (simulated) particle with density 1000 kg/m^3 is shown in Fig. 1c.

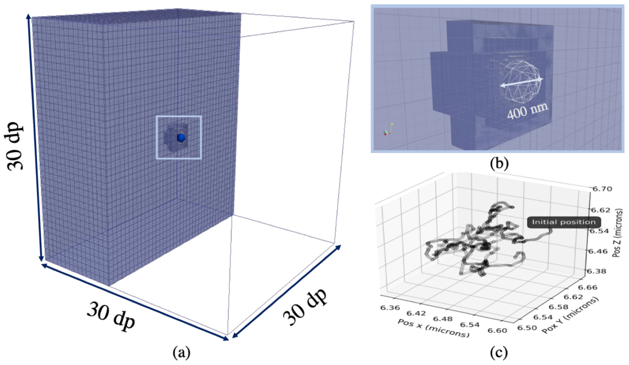

Figure 1: a) Schematic of the simulation domain, b) Octree-grid around the particle and c) Brownian trajectory of a 400 nm particle with density 1000 kg/m^3 after 100 response times

Several particle-fluid density ratios were simulated (ranging from 2000 to 100) in order to better understand the diffusion dynamics in such a system. The statistics from these Brownian diffusion simulations (non-dimensional mean squared displacements ($MSD/\sqrt{D\tau_p}$)) are averaged and compared with both Einstein's analytical diffusivity and a one-way coupled Lagrangian point-particle solution to Eq. 1. These Lagrangian simulations (for the same density ratio range) employ quasi-steady models such as the Stokes drag for the hydrodynamic coupling (Ounis & Ahmadi 1990) and are further ensemble averaged over 5 realizations. The current framework compares very well with these point-particle simulations, particularly at the chosen density ratios (c.f. Fig 2a), capturing the transition from a particle-inertia dominated (highly correlated) ballistic regime (t^2) to a non-correlated diffusive one (*2Dt*). The Gaussian nature of $F_{Brownian}$ in Eq. 1 would mean that the consequent stochastic process is Markovian in nature. Hence, the auto-correlation function (*Vacf*) of the particle velocity decays with an exponential tail, as shown in Fig 2b. This classical result for Brownian particles (Uhlenbeck & Ornstein 1930), with sufficiently high density ratios, is further a validation of the performance of our framework.

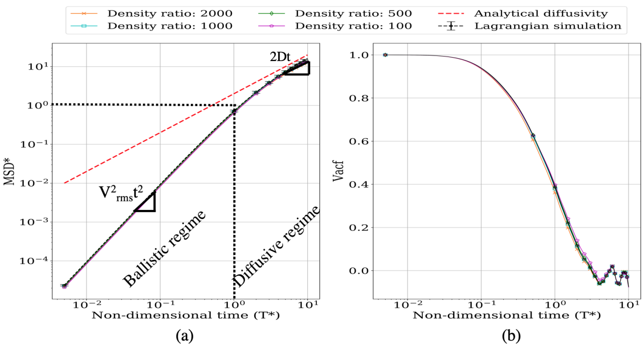

Figure 2: Comparison between the IB-FSI and Lagrangian simulations: a) Diffusion dynamics and b) averaged velocity auto-correlation function across different particle-fluid density ratios after 100 response times

Conclusions

In this paper, we have presented a simulation tool that extends the applicability of a fully resolved continuum description of a weakly rarefied gas to study the diffusion dynamics of a spherical HC nanoparticle in an unbounded domain. We have found this framework to be perfectly suited to study soot-like spherical particles at realistic density ratios. These simulations serve as the foundation to further extending our method for studying more complicated phenomena encountered in aerosol dispersions, such as wall interactions, multi-particle interactions etc., which are conventionally harder to probe using a purely Lagrangian description of the corresponding extended Langevin equations.

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